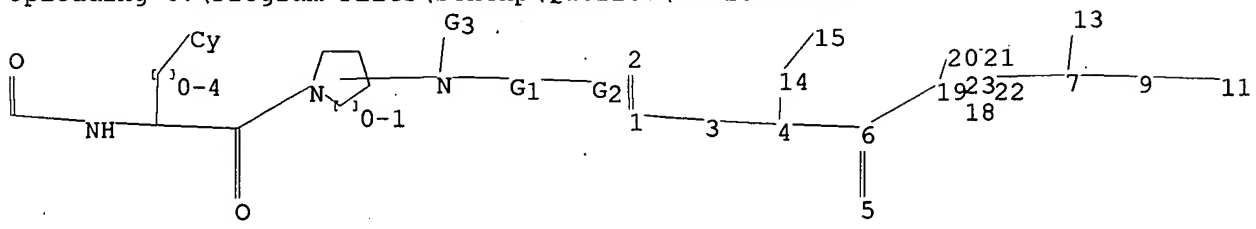
FILE 'HOME' ENTERED AT 13:47:23 ON 08 JUL 2005

=> file reg
Uploading C:\Program Files\Stnexp\Queries\10813870.str



chain nodes :
1 2 3 4 5 6 7 9 11 13 14 15
ring nodes :
18 19 20 21 22
chain bonds :
1-2 1-3 3-4 4-6 4-14 5-6 6-19 7-9 7-13 9-11 14-15
ring bonds :
18-19 18-22 19-20 20-21 21-22
exact/norm bonds :
1-2 1-3 3-4 5-6 6-19 7-9 7-13 9-11 14-15 18-19 19-20
exact bonds :
4-6 4-14 18-22 20-21 21-22
isolated ring systems :
containing 18 :

G1:C,S

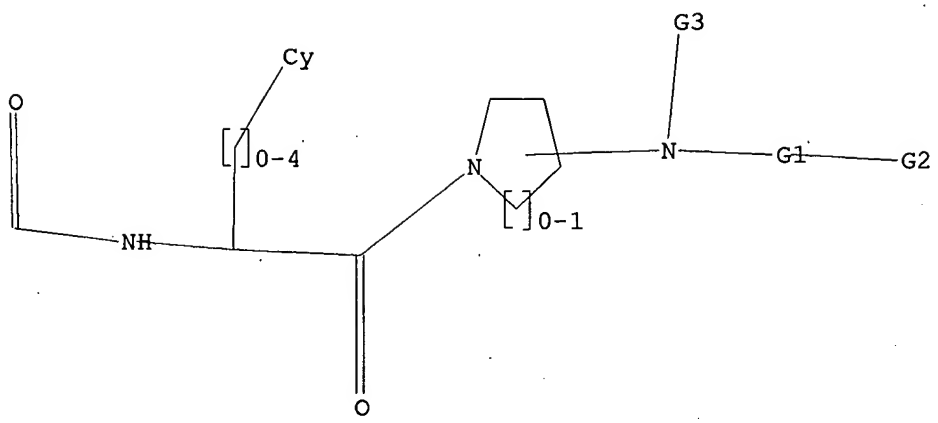
G2:Cy,Ak

G3:Cb,Ak

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS 11:CLASS
13:CLASS 14:CLASS 15:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS

L1 STRUCTURE UPLOADED

=> dis l1
L1 HAS NO ANSWERS
L1 STR



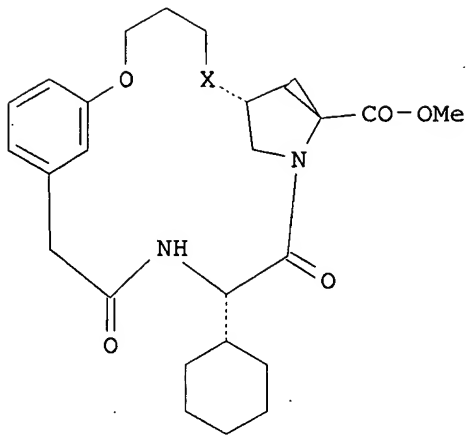
G1 C,S

G2 Cy,Ak

G3 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sam
L2             3 SEA SSS SAM L1

=> s l1 full
L3           207 SEA SSS FUL L1

=> file caplus
=> s l3
L4             5 L3

=> s l4 and pd<may 2003
      23381835 PD<MAY 2003
                (PD<20030500)
L5             2 L4 AND PD<MAY 2003

=> dis l5 1-2 bib abs hitstr

L5   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2002:312325  CAPLUS
DN   137:47431
TI   Novel Dipeptide Macrocycles from 4-Oxo, -Thio, and -Amino-Substituted
     Proline Derivatives
AU   Arasappan, Ashok; Chen, Kevin X.; Njoroge, F. George; Parekh, Tejal N.;
     Girijavallabhan, Viyyoor
CS   Schering Plough Research Institute, Kenilworth, NJ, 07033, USA
SO   Journal of Organic Chemistry (2002), 67(11), 3923-3926
     CODEN: JOCEAH; ISSN: 0022-3263
PB   American Chemical Society
DT   Journal
LA   English
OS   CASREACT 137:47431
GI
```



I

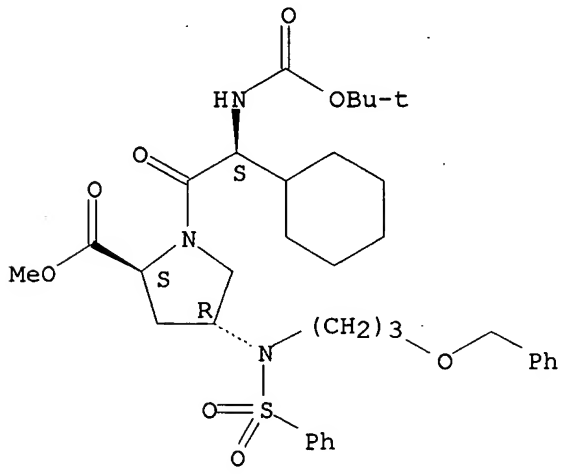
AB Dipeptide macrocycles [(I); X = O, S, N-SO2Ph] have been constructed in a versatile manner from the corresponding 4-heteroatom-substituted proline derivs. using an intramol. Mitsunobu strategy as the key step.

IT **367260-04-6P 367260-06-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of macrocyclic dipeptides via intramol. Mitsunobu cyclization)

RN 367260-04-6 CAPLUS

CN L-Proline, (2S)-2-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

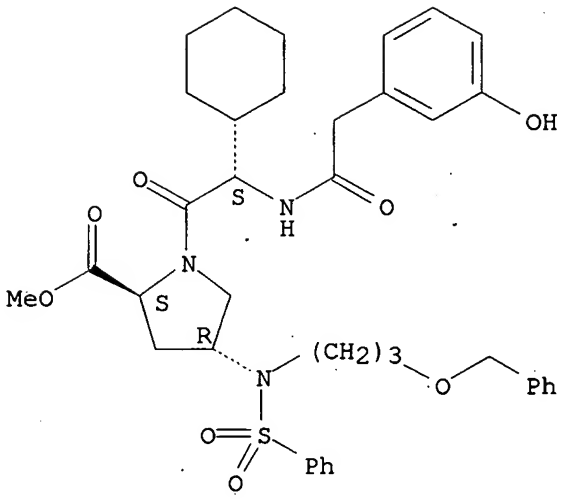
Absolute stereochemistry.



RN 367260-06-8 CAPLUS

CN L-Proline, (2S)-2-cyclohexyl-N-[(3-hydroxyphenyl)acetyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:763001 CAPLUS
DN 135:318715
TI Preparation of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising n-cyclic p2 moieties
IN Chen, Kevin X.; Arasappan, Ashok; Venkatraman, Srikanth; Parekh, Tejal N.; Gu, Haining; Njoroge, F. George; Girijavallabhan, Viyyoor M.; Ganguly, Ashit; Saksena, Anil; Jao, Edwin; Yao, Nanhua H.; Prongay, Andrew J.; Madison, Vincent S.; Vibulbhan, Bancha
PA Schering Corporation, USA
SO PCT Int. Appl., 402 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001077113	A2	20011018	WO 2001-US10869	20010403 <--
	WO 2001077113	A3	20020620		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2405521	AA	20011018	CA 2001-2405521	20010403 <--
	AU 2001053124	A5	20011023	AU 2001-53124	20010403 <--
	US 2002107181	A1	20020808	US 2001-825399	20010403 <--
	US 6846802	B2	20050125		
	EP 1268525	A2	20030102	EP 2001-926601	20010403 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

	BR 2001009861	A	20030610	BR 2001-9861	20010403
	JP 2003530401	T2	20031014	JP 2001-575586	20010403
	NZ 521455	A	20040625	NZ 2001-521455	20010403
	ZA 2002007845	A	20040211	ZA 2002-7845	20020930
	NO 2002004797	A	20021204	NO 2002-4797	20021004 <--
PRAI	US 2000-194607P	P	20000405		
	WO 2001-US10869	W	20010403		

OS MARPAT 135:318715

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

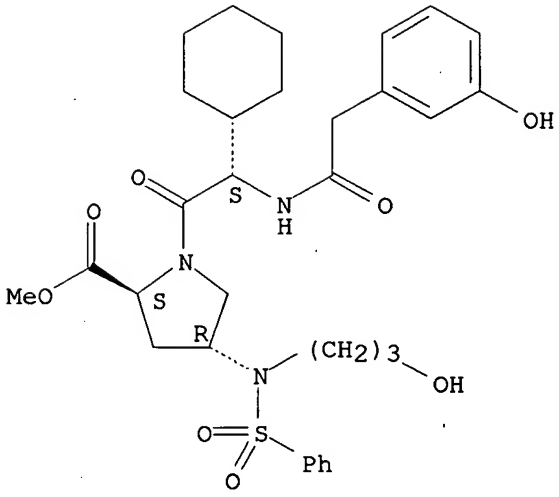
AB Title compds. I [wherein X and Y = independently (cyclo)alkyl, heteroalkyl, (aryl)heteroaryl, alkyl(hetero)aryl, substituted ether, sulfide, sulfone, amide, sulfonamide, urea, carbamate, hydrazide, carbonyl, etc.; R1 = CHO, acyl, or (un)substituted carboxy, carbamoyl, boryl, etc.; Z = O, N, or CH, W = null or CO, CS, or SO2; Q = null or CH, N, P, (CH2)p, (CHR)p, (CRR')p, O, NR, S, or SO2; A = O, CH2, (CHR)p, (CHRCHR')p, (CRR')p, NR, S, SO2, or a bond; E = CH, N, CR, or a double bond toward A, L, or G; G = null or (CH2)p, (CHR)p, or (CRR')p; J = null or CH, CR, O, S, or NR; M = null or O, NR, S, SO2, "(CH2)p, (CHR)p, (CHRCHR')p, or (CRR')p; p = 0-6; R, R', R2, R3, and R4 = independently H, (cyclo)alkyl, alkenyl, heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate, urea, ketone, CHO, CN, NO2, O, N, S, P, etc.] were prepared as hepatitis C virus (HCV) protease inhibitors. For example, II (multi-step preparation given) was cyclized, deesterified, and coupled with III•HCl (preparation given) to give the macrocyclic hydroxyamide intermediate. Oxidation using Des-Martin reagent followed by flash chromatog. afforded two diastereomers IV in 82% combined yield. The (S)-isomer inhibited NS3-serine protease HeLa/Huh7 co-transfected cells with a Ki of 2 μM. The invention also discloses pharmaceutical compns. comprising I as well as methods of using them to treat disorders associated with the HCV protease.

IT **367261-32-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)

RN 367261-32-3 CAPLUS

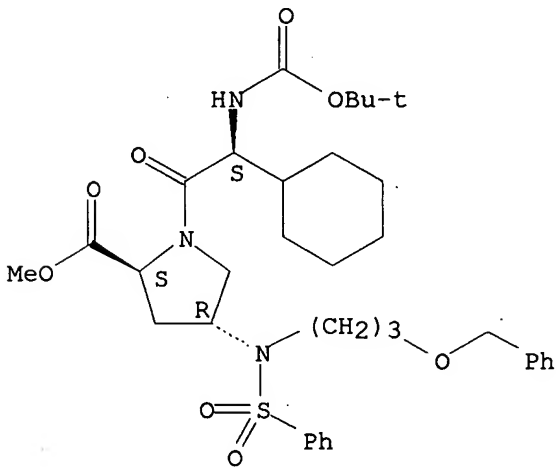
CN L-Proline, (2S)-2-cyclohexyl-N-[(3-hydroxyphenyl)acetyl]glycyl-4-[(3-hydroxypropyl)(phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



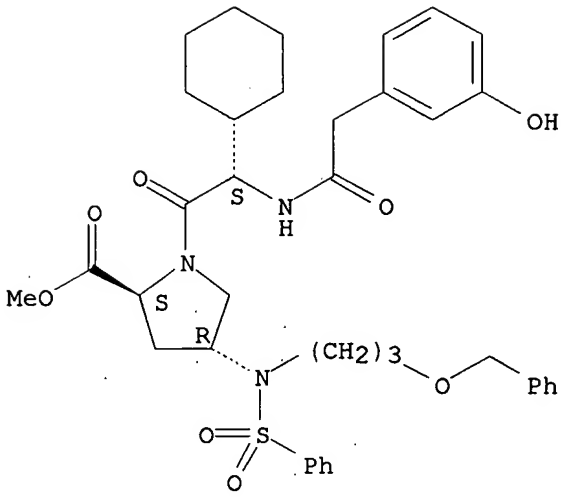
IT **367260-04-6P 367260-06-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of macrocyclic NS3-serine protease inhibitors of hepatitis C virus comprising cyclic p2 moieties)
RN 367260-04-6 CAPLUS
CN L-Proline, (2S)-2-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

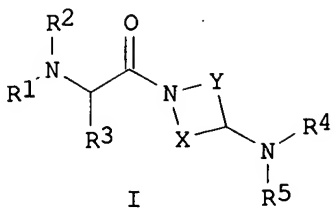


RN 367260-06-8 CAPLUS
CN L-Proline, (2S)-2-cyclohexyl-N-[(3-hydroxyphenyl)acetyl]glycyl-4-[[3-(phenylmethoxy)propyl](phenylsulfonyl)amino]-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=> s l4 not l5
L6             3 L4 NOT L5

=> dis l6 1-3 bib abs

L6   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2005 ACS on STN
AN   2005:451355  CAPLUS
DN   143:7980
TI   Preparation of amino acid aminoheterocyclyl amides as melanocortin
     receptor agonists
IN   Lee, Koo; Park, Heui-Sul; Ahn, In-Ae; Yoo, Hyun-Ju; Kim, Jong-Yup; Choi,
     Deog-Young; Yim, Hyeon-Joo; Chung, Kyung-Ha; Shim, Dong-Sup; Lee,
     Sang-Kyun; Kondoh, Yutaka; Hirabayashi, Ryoji; Honda, Shugo; Kaku,
     Hidetaka; Shishikura, Jun-ichi; Ito, Hiroyuki; Kurama, Takeshi
PA   Lg Life Sciences Ltd., S. Korea; Yamanouchi Pharmaceutical Co., Ltd.
SO   PCT Int. Appl., 117 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.          DATE
     ---------------     ----   --------    --------------------     --------
PI   WO 2005047251        A1     20050526    WO 2004-KR2929           20041112
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO,
             SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
PRAI KR 2003-79799        A      20031112
     KR 2004-65820        A      20040820
GI
```



I

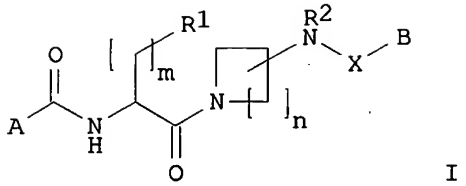
AB The invention relates to amino acid derivs. I [X, Y = CH2 or CH2CH2; R1 = H, (CH2)0-3-R6, (CH2)0-3CO(CH2)0-3-R6, (CH2)0-3SO2(CH2)0-3-R6, etc., where R6 = (un)substituted alkyl, alkoxy, cycloalkyl, heterocyclyl, aryl, heteroaryl, amino or hydroxy; R2 = H, (un)substituted alkyl, cycloalkyl or CO(CH2)0-3-R6; R3, R4 = H, alkyl, (CH2)0-3-cycloalkyl, -aryl, -heteroaryl or -heterocyclyl in which the rings may be substituted; R5 = H, alkyl, or (CH2)0-3 substituted by acyl, (thio)carbamoyl, sulfamoyl or sulfonyl groups; or R1R2N, R4R5N = heterocyclyl], including pharmaceutically-acceptable salts, hydrates, solvates and isomers, which are effective agonists of the melanocortin receptor (MCR). Thus, (2R)-2-amino-N-[(3S)-3-[cyclohexyl(isobutyryl)amino]pyrrolidine-1-yl]-3-(4-chlorophenyl)propionamide TFA salt was prepared via amidation reaction and showed EC50 = 0.005-0.5 μM and IC50 = 0.1-0.5 μM against MCR4.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

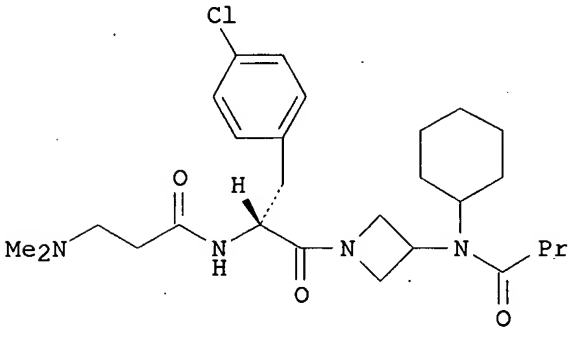
L6 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:964812 CAPLUS
DN 141:411215
TI Preparation of amino acid heterocyclyl amides as modulators of the melanocortin-4 receptor
IN Chaturvedula, Prasad V.; Luo, Guanglin; Vig, Shikha; Poindexter, Graham S.; Beno, Brett R.
PA USA
SO U.S. Pat. Appl. Publ., 31 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004224901	A1	20041111	US 2004-813870	20040330
PRAI	US 2003-465552P	P	20030425		

OS MARPAT 141:411215
GI



I



II

AB Novel azetidinyl and pyrrolidinyl compds. I [A is H, alkyl, aminoalkyl, optionally N-alkylated azetidinyl, pyrrolidinyl, piperidinyl, piperazinyl, (thio)morpholinyl or (iso)quinolinyl; R1 is (un)substituted Ph, naphthyl, benzofuranyl, benzothienyl or indolyl; R2 is alkyl or cycloalkyl; m is 0-3; n is 1 or 2; X is CO or SO2; B is alkyl, cycloalkyl, cycloalkylmethyl, methoxy- or phenoxyalkyl, (un)substituted Ph, naphthyl, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, furanyl, thienyl, pyrrolyl, oxazolyl, isoxazolyl, benzfuranyl, benzthienyl, indolyl, benzoxazolyl or indazolyl] and their pharmaceutically-acceptable salts are ligands of melanocortin-4 receptors (MC4R) and are useful for treating conditions responsive to the modulation of melanocortin-4 receptors such as obesity, diabetes, and sexual dysfunction. Thus, 4-chlorophenylalanyl azetidine derivative II was prepared via acylation reactions and showed IC50 < 250 nM in the MC4R binding assay.

L6 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:370923 CAPLUS
DN 140:391302
TI Preparation of benzo-1,3-diazepin-2-ones and related compounds as CGRP receptor antagonists for the treatment of migraine headaches
IN Rudolf, Klaus; Mueller, Stephan Georg; Stenkamp, Dirk; Lustenberger, Philipp; Dreyer, Alexander; Bauer, Eckhart; Schindler, Marcus; Arndt, Kirsten; Doods, Henri
PA Boehringer Ingelheim, Germany
SO PCT Int. Appl., 254 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004037811	A1	20040506	WO 2003-EP11763	20031023
	WO 2004037811	C1	20050519		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,

GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

DE	10250082	A1	20040513	DE 2002-10250082	20021025
US	2004132716	A1	20040708	US 2003-685921	20031015
PRAI DE	2002-10250082	A	20021025		
US	2002-426167P	P	20021114		

OS MARPAT 140:391302
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = O, S, phenylsulfonylimino, etc.; X = O, S, substituted imino, etc.; Y, Z = alkyl, difluoromethyl, trifluoromethyl, etc.; R1 = 5-7 membered aza, diaza, triaza, etc. heterocycle; R2 = H, phenylmethyl, alkyl, etc.; R3 = H, Ph, pyridinyl, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, benzo-1,3-diazepin-2-one II was prepared from 1-(3,4-diethylphenyl)ethanone in 8-steps. In human CGRP receptor binding affinity assays, compds. I exhibited IC50 values < 10000 nM. Compds. I are claimed useful for the treatment of migraine headaches.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	20.62	183.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.65	-3.65

STN INTERNATIONAL LOGOFF AT 13:49:37 ON 08 JUL 2005